

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:1078234 CAPLUS Full-text

DN 143:347210

TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents

IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajashekhar

PA Council of Scientific and Industrial Research, India

SO U.S. Pat. Appl. Publ., 13 pp.

CODEN: USXXCO

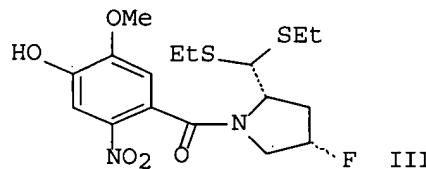
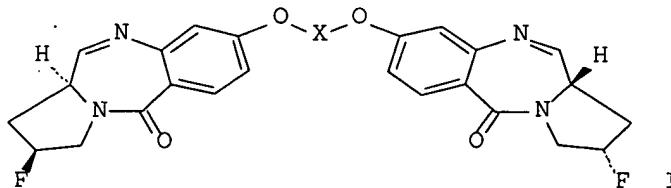
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005222131	A1	20051006	US 2004-812840	20040330
PRAI	US 2004-812840		20040330		

GI



AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH₂)₃₋₁₀], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = (CH₂)₄; logGI50 = -5.21, logTGI50 = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.

IT 717920-82-6P 717920-83-7P 717920-84-8P

858639-17-5P 858639-19-7P 858639-21-1P

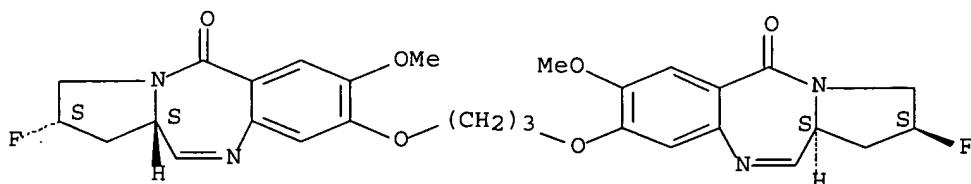
858639-23-3P 858639-25-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)

RN 717920-82-6 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-(1,3-propanediylbis(oxy))bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

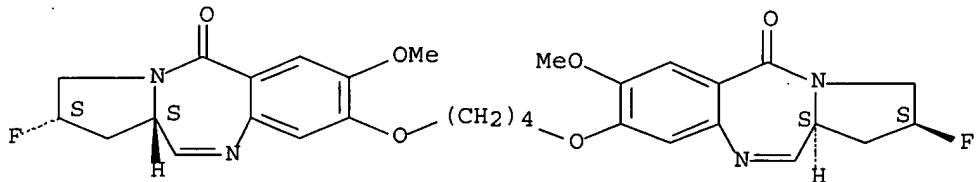


RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-(1,4-butanediylbis(oxy))bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-,

(2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

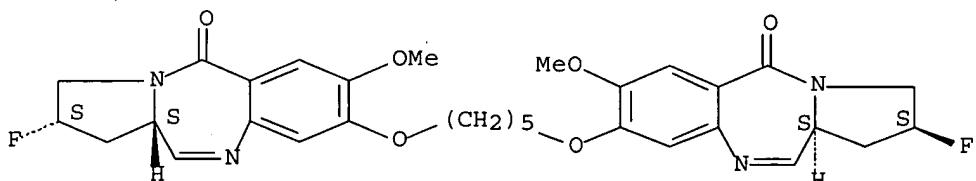
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediylibis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

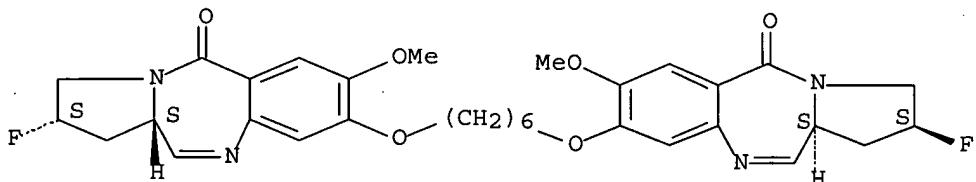
Absolute stereochemistry.



RN 858639-17-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediylibis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

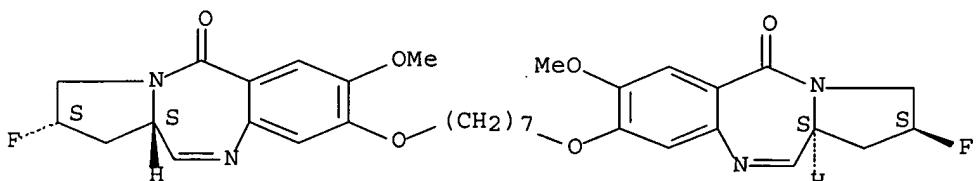
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediylibis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

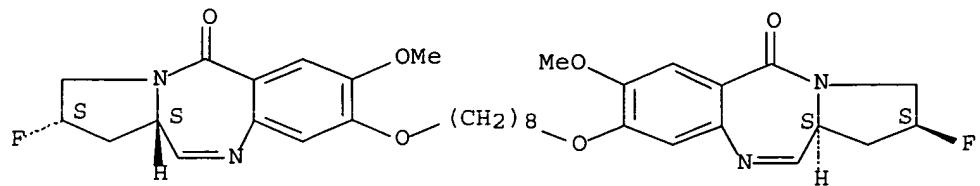
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediylibis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

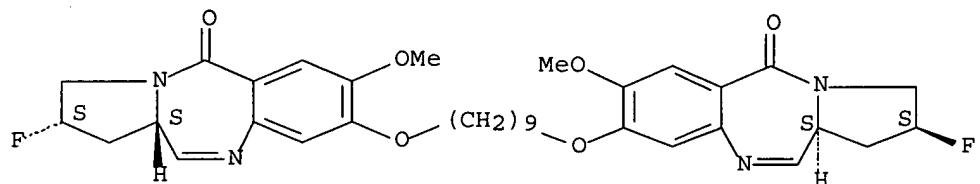
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

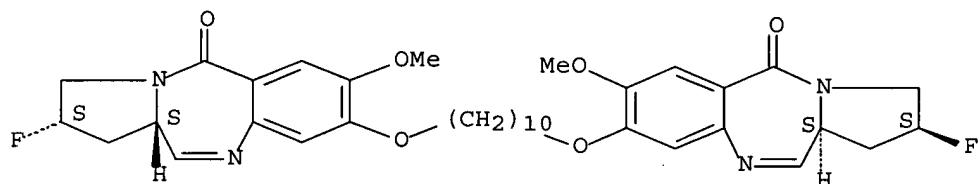
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:612296 CAPLUS Full-text

DN 143:133404

TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents

IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajasekhar

PA Council of Scientific and Industrial Research, India

SO PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DT Patent

LA English

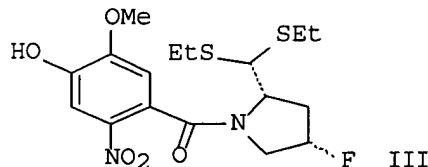
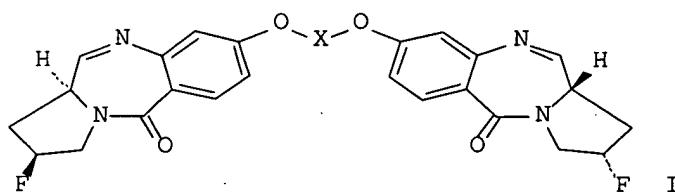
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005063758	A1	20050714	WO 2003-IN448	20031231
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PRAI WO 2003-IN448 20031231

OS CASREACT 143:133404

GI



AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH₂)₃₋₁₀], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = CH₂)₄; (logGI50 = -5.21, logTGI50 = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.

IT 717920-82-6P 717920-83-7P 717920-84-8P

858639-17-5P 858639-19-7P 858639-21-1P

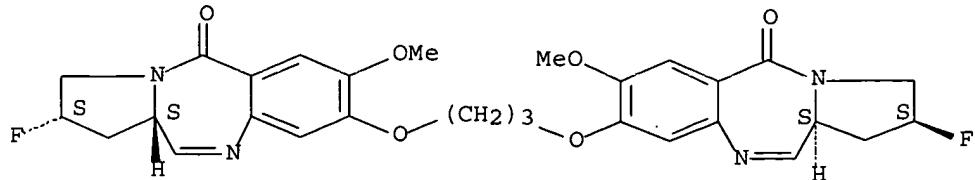
858639-23-3P 858639-25-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)

RN 717920-82-6 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

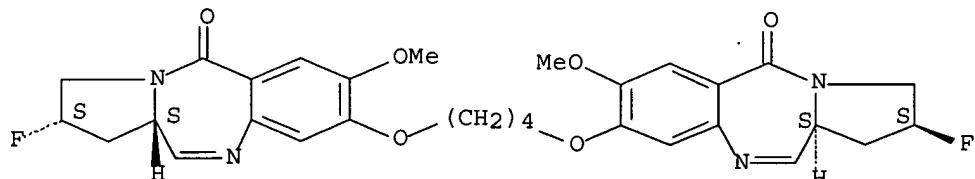
Absolute stereochemistry.



RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

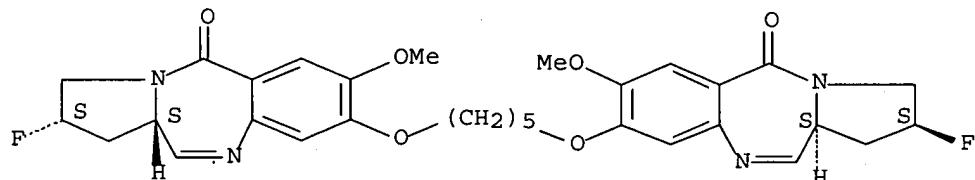
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

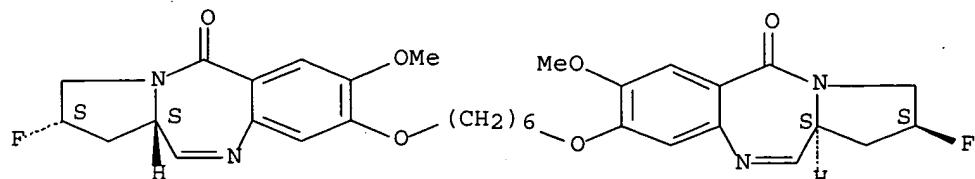
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CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

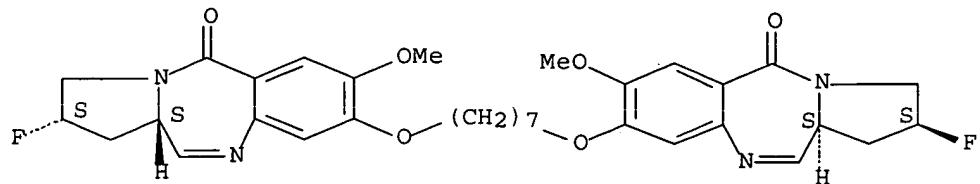
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

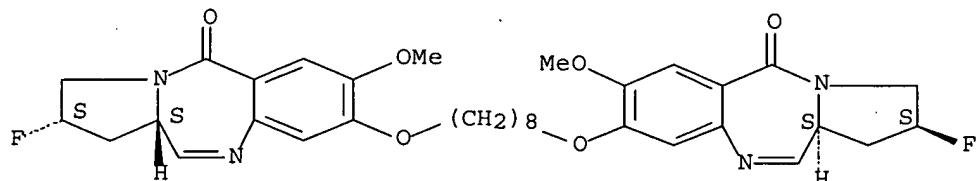
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

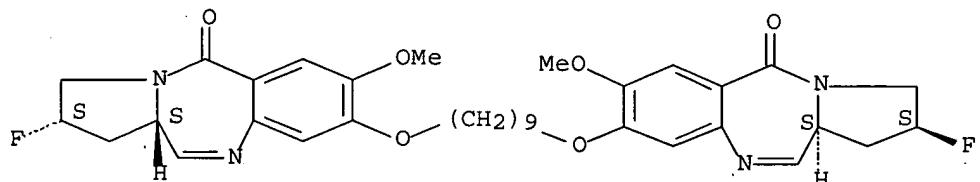
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

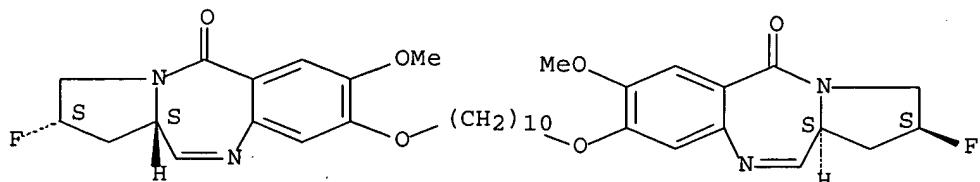
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

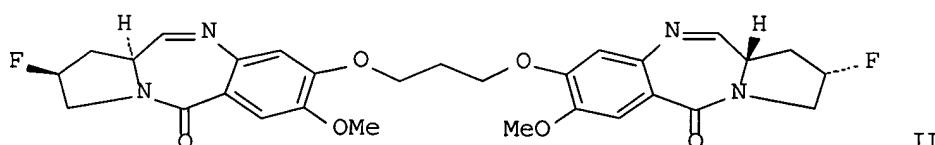
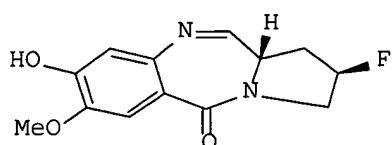
Absolute stereochemistry.



RE.CNT 4

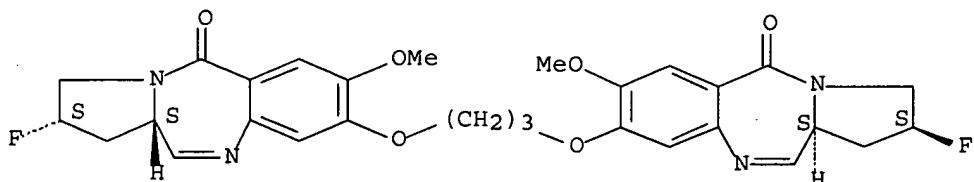
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

LS ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:346285 CAPLUS Full-text
 DN 141:106440
 TI The effect of C2-fluoro group on the biological activity of DC-81 and its dimers
 AU Kamal, Ahmed; Reddy, P. S. M. M.; Reddy, D. Rajasekhar
 CS Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500007, India
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2669-2672
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science B.V.
 DT Journal
 LA English
 OS CASREACT 141:106440
 GI



AB C2-Fluoro substituted pyrrolobenzodiazepines were synthesized that exhibit potential anticancer activity in a number of human tumor cell lines. These C2-fluoro substituted PBDs also exhibit significant DNA-binding ability. Example compds. included (2R,11aS)-2-Fluoro-1,2,3,11a-tetrahydro-8-hydroxy-7-methoxy-5H-pyrrolo[2,1-c][1,4]benzodiazepin-5-one (I) and a dimer (II).
 IT 717920-82-6P 717920-83-7P 717920-84-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of (fluoro)tetrahydro(hydroxy)pyrrolo[2,1-c][1,4]benzodiazepin-5-one derivs. and dimers and study of their anticancer activity)
 RN 717920-82-6 CAPLUS
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-(1,3-propanediylbis(oxy))bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)-(9CI) (CA INDEX NAME)

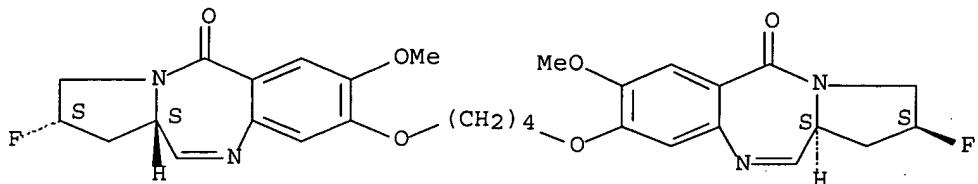
Absolute stereochemistry.



RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

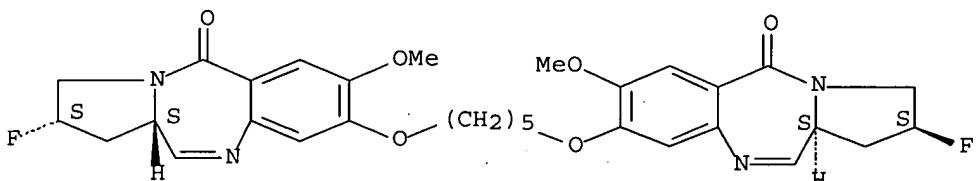
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-(pentanediylbis(oxy))bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 8 S L2 FUL

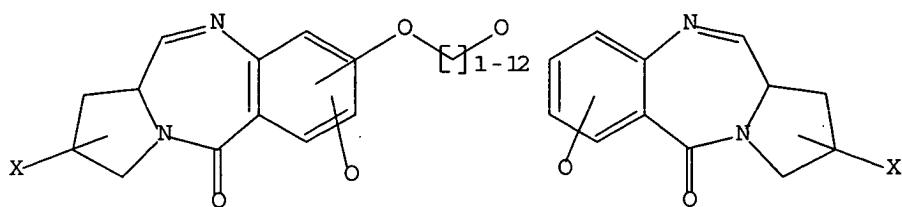
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L2 HAS NO ANSWERS

L1 STR



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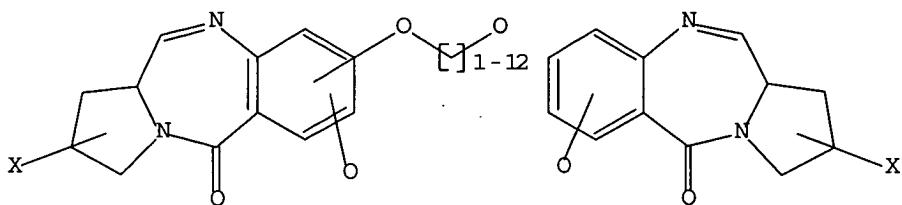
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 L3 1 S L2
 L4 8 S L2 FUL

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L5 3 S L4

=> d l2; d his; log y
 L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.
 L2 QUE ABB=ON PLU=ON L1

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FILE 'REGISTRY' ENTERED AT 09:34:02 ON 27 JAN 2006

L1 STRUCTURE UPLOADED
 L2 QUE L1
 L3 1 S L2
 L4 8 S L2 FUL

FILE 'CAPLUS' ENTERED AT 09:34:28 ON 27 JAN 2006
L5 3 S L4

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FULL ESTIMATED COST	15.79	182.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

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